

Quantitative Assessment of the Atom Radii of Chemical Elements Based on Spectral Analysis Data

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Abstract— Atom radii are calculated for chemical elements in different energy states based on photon energy of the emission (absorption) spectrum of atoms.

Keywords: atom, radius, emission spectrum, photon

I. INTRODUCTION

The term *nanotechnology* stands for a set of methods and techniques used to create materials with dimensions in the nanometre scale (at atomic and molecular levels) in order to produce new products with predetermined properties. Other well-known concepts include *molecular nanotechnology* (MNT) by K. E. Drexler [1-3], *submicron nanosystem technology* by N. Taniguchi [4], the molecular building block method [5-8] and *in-between level nanotechnology*. Development of nanotechnology as a scientific theory can be proved only if nanodevices are made available. In case of the molecular building block method, nanodevices are assembled from chemically pre-synthesized molecules (carbon-bearing building blocks that also include nitrogen, boron, etc.) that are capable of forming bonds with each other [5-8]. Such dimensions are typical for the main biological structures: cells, their components (organelles) and molecules, complex inorganic compounds examined in recent scientific publications [9-11]. Taking into account significance and rapid advancement of nanotechnologies, we decided to provide a quantitative assessment of atom radii for different chemical elements in this publication.

A radius of the atom is one of the most important parameters that determines its length and, as a result, the strength of chemical bonds between atoms in molecules, as well as the efficiency of different technological processes. Therefore, quantitative assessment of atom radii for different chemical elements depending on their energy state is significant both from theoretical and practical point of views.

II. DIFFERENT CONCEPTS OF AN ATOMIC RADIUS

To define a radius of the atom, a number of concepts are applicable depending on the modeling paradigm, classical or quantum mechanical one: atomic, orbital, effective, covalent, or van der Waals radius. In the N. Bohr model of the atom, where electrons travel in defined circular orbits (i.e. energy levels), the *radius of the atom is the distance from the center of the nucleus to the furthest electron orbit*. An *atomic radius* is a characteristic of an atom that allows for an approximate estimation of interatomic (inter-nuclear) distances in molecules and crystals [12, 13]. An *orbital radius* of an atom is theoretically calculated as a distance from the nucleus to the maximum in the radial probability distribution curve for the electron density in an atom, i.e. it is a characteristic of the free atom sizes [13-15]. For various quantum-chemical calculations, values for orbital radii can differ.

The *effective radius* of an atom is estimated according to its sphere of action in the compound. It depends on its action manifestation, i.e. it is a characteristic of atoms in molecules bound together in a crystal structure. The radius value depends on the atom environment and interactions, as well as the state of atoms in the crystal structure. It is measured using X-ray data and is based on inter-nuclear distances. Otherwise, electron density distribution maps can be used and the radius is calculated as a distance from the nucleus to the electron density minimum along a bond line.

The concepts of orbital and effective [14, 15] radii are based on solutions to the Schrödinger's equation and assume the wave-particle duality of electrons moving in a hydrogen atom. The radius of the hydrogen atom is determined by atomic orbital types that significantly differ: s, p, d, h, f, etc. Therefore, according to the wave properties of an electron,

atoms do not have strict boundaries and the concept of *the atomic radius* implies that 90-98% of the electron density lies within this sphere. It should be emphasized that the Schrödinger's equation describes the motion of a single electron in a hydrogen atom or a hydrogen-like ion. However, it is currently used for multi-electron atoms as well. For example, B. F. Bratsev [16] considers atom wave function for atom states from helium to argon. To calculate them, he uses the quantum theory of the atom with the Hartree-Fock approximation. During the last decade a number of research papers offered a more critical approach to the Schrödinger's theory [17-19].

Depending on the atom bond type, metal, covalent and van der Waals atomic radii are also distinguished [15]. A *metal radius* is half the shortest distance between two atoms between atoms in the metal crystal structure. The value depends on the number of neighbors in the structure around the atom in the structure (i.e. coordination number). A *covalent radius* is half the length of a single chemical bond X—X, where X is a nonmetal atom. For halogen, the covalent atomic radius is half the internuclear distance in the X₂ molecule.

The size of an atom is determined by its electron shell. However, the shell is not limited to a strict defined surface. The effective radius of the atom is specified by the *van der Waals radius*. It specifies the minimum possible distance-dependent interactions for atoms that belong to different molecules. Thus Van der Waals radius equals half the internuclear distance between the nearest identical atoms that are not connected by chemical bonds, i.e. belong to different molecules. These radii determine the effective size of noble gas atoms [20].

III. EXISTING METHODS FOR DETERMINING ATOM RADII

In 1911 E. Rutherford experimentally proved the planetary model of the atom, while N. Bohr introduced a theoretical model for it together with a formula for calculating chemical element atom radius [21]:

$$r_n = n^2 \frac{\hbar^2 4\pi \epsilon_0}{m_e Z e^2} = 0.529 \cdot 10^{-10} \frac{n^2}{Z}, \quad (1)$$

where n is the main quantum number that can take integer values from 1 to ∞ ; m_e is electron mass; e is electron charge; Z is a number of protons in the atom nucleus or the atomic number of a chemical element in the Mendeleev's periodic table; ϵ_0 is an electric constant or a vacuum permittivity constant; $\hbar = \frac{h}{2\pi}$; h is a Planck constant.

As this formula shows, radii of atoms (outermost electron orbits) increase in proportion to the integer squares. For the hydrogen atom ($Z = 1$), the radius of the first electron orbit when $n = 1$ is called the Bohr radius and equals $0.529 \cdot 10^{-10}$ m. This value is considered to be a close approximation of reality. However, there is a drawback to the equation (1): the size of the atom radii of chemical elements increases drastically if n

parameter increases. According to it, if $n = \infty$ then $r = \infty$, which makes no physical sense. In addition, in the equation (1) for a valence electron only the net positive charge is considered via Z variable. It does not take into account the distribution of energy as a nucleus interacts with all atom's electrons and electron shielding effect in polyelectronic atoms. Therefore, the equation (1) can actually be used only to calculate the hydrogen atom radius by $n = 1 \div 7$.

There is another method for assessing atom radii for chemical elements [12]. It uses a bulk density value for a substance composed of these elements and takes into account the estimated coordination number and crystal lattice structures:

$$r = \sqrt{\frac{3 \cdot \mu \cdot (1 - K_{na})}{4 \cdot \rho \cdot N_a}}, \quad (2)$$

where ρ is the bulk density of the substance ($\frac{kg}{m^3}$);

μ is the molar mass ($\frac{kg}{mole}$);

K_{na} is interatomic porosity expressed as a decimal fraction;

N_a is the Avogadro's number ($N_a = 6,022 \cdot 10^{23}$ atoms/mole).

Atom radii for many chemical elements were calculated using the equation (2) by different authors (L. Pauling, N. No. Belov and G. Bokiia and others) and can be found in a book by T. Goronovsky et al. [12] according to their coordination numbers. This method of calculation has its drawback: there is no data on the densities and types of crystal structures, i.e. a reliable estimate for the K_{na} parameter of substances composed from different chemical elements in different energy states.

In a research [14] it is noted that there exist around 20 systems of values of effective radii for atoms and ions. These systems are based on two established approaches. The first approach assumes that a radius of the oxygen ion is greater than the radius of main cations. It was suggested by A. Lande in the 1920s and is based on the additivity principles (i.e. internuclear distance is the sum of the radii of atoms or ions) and densest packing of atoms in crystals (anion spheres touch each other). Anion radius is defined as half the shortest distance between anions. Based on internuclear distances in some selenides and sulfides, radius values were calculated for S₂—0.183 nm, Se₂—0.193 nm, Mg₂₊ (0.076 nm). Later in 1926 V. Goldschmidt created a radius system for ions of all chemical elements. For reference values, he used an anion radius of fluorine (0.133 nm) and oxygen (0.132 nm). These values were calculated using a refractometric method by D. Vazasherna in 1923 (based on refraction indices of fluoride in aqueous solutions). Later this system of radii was elaborated by N. Belova, G. Bokiia, L. Pauling, R. Shanon, K. Prewitt and others. In the Pauling system, the O₂ radius is 0.140 nm, in the Bokiia–Belov system it is 0.136 nm.

The second approach was developed by W. L. Bragg in 1920 as he analyzed crystal structure by means of X-ray. As a reference value, he uses the radius of sulfidion (0.103 nm) that was defined based on internuclear distance S—S (0.205 nm) in pyrite (FeS_2) via radiographic measurement techniques. The principles of calculating radii of ions for all other elements stayed the same as in the first approach. However, he assumed the radii of oxygen and sulfur anions to be smaller than the radii of cations, i.e. the densest packing is formed by cations while anions fill in the voids.

Radius systems are constantly refined and revised. In the periodic table of chemical elements, values of the orbital radii for atoms are often specified. They are results of theoretical calculations of electron density distribution in isolated atoms. These values usually provide the foundation to establish patterns of atom radius change between chemical element of different groups and periods in the periodic table. For example, data on the atomic radius values can be found in a reference book *Physical quantities* [22]. However, researches made by different authors, as well as data from the periodic table, do not cover a lot of chemical elements when it comes to their atom radii (for example, promethium, astatine, elements from americium to einsteinium and mendelevium). Therefore, the quantitative assessment of atom radii for chemical elements based on spectral analysis across the whole energy range of atoms significantly expands the possibilities for researching and solving this issue.

IV. VALIDATION OF A NEW METHOD OF QUANTITATIVE ASSESSMENT OF ATOM RADII FOR CHEMICAL ELEMENTS DEPENDING ON THEIR ENERGY STATE

A research [23] for the first time offers and validates the use of a mathematical expression for quantitative assessment of atom radii for chemical elements in various energy states based on spectral analysis data. It uses a proton-electron-photon model of the atom structure of the atom that was researched in [18, 19]. It takes into account that photons present in the atom have a definite emission-absorption spectrum, which is directly related to the problem considered in this paper.

Here, we assume that photons actually exist in the atom structure rotating around external electrons and nucleons. The photon spectrum of a particular atom is determined by the presence of photons forming a photon field around each charged particle of the atom. Each electron of an atom is characterized by a specific photon spectrum.

The atom spectrum is the spectrum of all photons emitted or absorbed by the valence (least bound) electron of a given atom. The atom absorbs the same spectrum as the emitted one. Therefore, spectral analysis can be used to determine the presence of certain elements in a substance. In accordance with this principle, hydrogen has six series in the spectrum due to photon emission-absorption. They represent six photon orbitals around the hydrogen atom electron. The presence of a photon electromagnetic field around all charged particles in an atom and interaction of electrons with an atom nucleus via fields stabilizes of the atom. Otherwise, according to the laws of electrodynamics, electrons moving in a circular orbit with centripetal acceleration would have been

continuously losing energy and as a result would have fallen to the nucleus. This view conforms with the Bohr's theory in the part where an electron moves in one circular orbit until it jumps to another. However, Bohr states that "the emission of photons occurs when electrons jump from one energy level to another," i.e. it is the transition of electrons that is initial. We cannot agree with Bohr's viewpoint. Since a photon is initial in the emission process, then it is the photons that are absorbed or emitted by the atom for it to be stable in its environment. Researches [23, 24] show that when photons are emitted and e^- jumps to an orbit closer to the nucleus, the emitted photons create a torque moment for e^- to rotate around the atom nucleus. This allowed authors to validate the mathematical expression of the electron rotation radius by emission of a photon of the corresponding frequency and energy.

$$r_i = \frac{\xi \cdot e^2}{8\pi^2 \cdot \epsilon_0 h \cdot v_i} = \frac{\xi \cdot e^2 \cdot \lambda_i}{8\pi^2 \cdot \epsilon_0 h \cdot c} \quad \text{therefore,}$$

$$r_i = 5,55 \cdot 10^4 \frac{\xi}{v_i} = 1,85 \cdot 10^{-4} \cdot \xi \cdot \lambda_i \quad (3)$$

e is electron charge ($e = 1,6 \cdot 10^{-19} \text{ C}$);

ϵ_0 is a vacuum permittivity constant ($\epsilon_0 = 8,85 \cdot 10^{-12} \frac{F}{m}$);

h is a Planck constant ($h = 6,626 \cdot 10^{-34} \text{ J}\cdot\text{s}$);

λ_i , v_i is length and frequency of the wave emitted by the atom of the i -th photon in the emission spectrum;

c – is the speed of light ($c = 2,997 \cdot 10^8 \text{ m/s}$);

$\xi = \frac{F_{ion}}{F_c}$ is the ratio of atom ionization force (F_{ion}) to the

coulombic attraction force (F_c) of the electron and a nucleus assuming that only one proton of the nucleus has influence. The ratio value varies from 0.45 to 1.15. The most probable value is within the range of 0.75-0.8 [23, 24]. Therefore, for most elements when calculating the force of electron–nucleus interaction, one can use the value $\xi = 0.75$ or a specific ξ value calculated for the element.

This approach can be used to assess atom radii for chemical elements across the entire energy range, i.e. in a wide range of temperatures. Thus, using the proposed method, we have calculated the atom radii for all chemical elements across their entire energy state range, which distinguishes this work from those of other authors (V. Brattsev [16], A. Radtsig and V. Shustriakov [22], L. Pauling, N. Belov and G. Bokiiu [12] and others).

V. PRACTICAL IMPLEMENTATION OF QUANTITATIVE ASSESSMENT OF ATOM RADII FOR CHEMICAL ELEMENTS BASED ON SPECTRAL ANALYSIS DATA

As examples of assessment of atom radii of chemical elements in different energy states, Table 1 offers results of radius calculations for a mercury atom using formula (3). The

calculations were made for all wavelengths of the emitted photons according to the tables of spectral lines [25].

$$\xi = \frac{F_{ion}}{F_C} = \frac{e \cdot \varphi_{ion} \cdot 4\pi \varepsilon_0 r^2}{r \cdot e^2} = \frac{\varphi_{ion} \cdot 4\pi \varepsilon_0 r}{e} \quad (4)$$

$$\xi = \frac{10.437 \cdot 4 \cdot 3.14 \cdot 8.85 \cdot 10^{-12} \cdot 1.57 \cdot 10^{-10}}{1.6 \cdot 10^{-19}} = 1.14$$

where $\varphi_{ion} = 10.437$ eV is ionization potential for the mercury atom; $e = 1.6 \cdot 10^{-19}$ C; $\varepsilon_0 = 8.85 \cdot 10^{-12} \frac{F}{m}$; $r = 1.57 \cdot 10^{-10}$ m is the mercury atom radius according to the data by Radtsig and V. Shustriakov [22].

TABLE I. CALCULATION OF MERCURY ATOM RADII ACROSS THE WHOLE RANGE OF ENERGY STATES

Emission wavelength $\lambda_i, \text{\AA}$	Atom radius $r, \text{\AA}$						
1	2	1	2	1	2	1	2
45122.04	9.4969	11206.0	2.3585	4991.5	1.0506	2803.47	0.5900
39283.61	8.2681	11176.8	2.3524	4916.07	1.0347	2799.76	0.5893
36303.03	7.6407	10715.5	2.2553	4890.27	1.0292	2759.71	0.5808
32148.06	6.7663	10432.0	2.1956	4827.1	1.0160	2752.78	0.5794
23253.07	4.8941	10423.5	2.1938	4358.33	0.9173	2699.51	0.5682
22493.28	4.7341	10359.5	2.1804	4347.49	0.9150	2698.83	0.5680
19700.17	4.1463	10333.0	2.1748	4343.63	0.9142	2655.13	0.5588
18130.38	3.8158	10298.2	2.1675	4339.22	0.9133	2653.68	0.5585
17436.18	3.6698	10229.6	2.1530	4108.05	0.8646	2652.04	0.5582
17329.41	3.6473	10139.79	2.1341	4077.83	0.8583	2625.19	0.5525
17213.20	3.6229	10129.7	2.1320	4046.56	0.8517	2603.15	0.5479
17206.15	3.6214	10121.2	2.1302	3906.37	0.8222	2576.29	0.5422
17198.67	3.6198	7728.82	1.6267	3801.66	0.8001	2536.52	0.5339
17116.75	3.6025	7091.86	1.4926	3704.17	0.7796	2534.76	0.5335
17109.93	3.6011	7081.9	1.4905	3701.44	0.7790	2483.82	0.5228
17072.79	3.5933	6907.46	1.4538	3663.28	0.7710	2482.71	0.5225
16942.00	3.5658	6716.43	1.4136	3662.88	0.7709	2482.00	0.5224
16933.27	3.5639	6234.4	1.3121	3654.84	0.7692	2464.06	0.5186
16920.16	3.5611	6072.72	1.2781	3650.15	0.7682	2399.73	0.5051
16881.48	3.5530	5871.97	1.2359	3341.48	0.7033	2399.35	0.5050
15295.82	3.2193	5859.25	1.2332	3144.48	0.6618	2379.99	0.5009
13950.55	2.9361	5803.78	1.2215	3135.76	0.6599	2378.32	0.5006
13673.51	2.8778	5790.66	1.2188	3131.84	0.6592	2374.02	0.4997
13570.21	2.8561	5789.66	1.2185	3131.55	0.6591	2352.48	0.4951
13505.58	2.8425	5769.60	1.2143	3125.67	0.6579	2345.43	0.4936
13468.38	2.8347	5675.86	1.1946	3027.49	0.6372	2323.20	0.4890
13426.57	2.8259	5549.63	1.1680	3025.61	0.6368	2302.06	0.4845
13209.95	2.7803	5460.73	1.1493	3023.48	0.6363	2002.00	0.4214
12071.7	2.5407	5384.63	1.1333	3021.50	0.6359	1972.94	0.4152
12020.0	2.5298	5354.05	1.1269	2967.28	0.6245	1849.50	0.3893
11977.3	2.5209	5290.74	1.1135	2925.41	0.6157	1832.60	0.3857
11769.1	2.4770	5218.9	1.0984	2893.59	0.6090	1775.68	0.3737
1168.7	2.4601	5137.94	1.0814	2856.94	0.6013	1774.90	0.3736
11491.7	2.4186	5120.63	1.0777	2847.83	0.5994	1250.59	0.1847
11372.5	2.3935	5102.71	1.0740	2806.77	0.5907		
11287.4	2.3756	5025.64	1.0577	2804.43	0.5902		

To confirm validity of the calculated results of mercury atom radii across a wide range of energy states, they are compared to mercury atoms radii calculated based on density values at three temperature states according to the data provided by P. Babicheva [22]. Density of mercury ρ :

$$\text{at } t = -39.9^\circ\text{C} \text{ it is equal to } 14.193 \cdot 10^3 \frac{\text{kg}}{\text{m}^3},$$

$$\text{at } t = 0^\circ\text{C} \text{ it is equal to } 13.59503 \cdot 10^3 \frac{\text{kg}}{\text{m}^3},$$

and at $t = 800^\circ\text{C}$ it is equal to $11.584 \cdot 10^3 \frac{\text{kg}}{\text{m}^3}$.

Radii of mercury atoms based on density at different temperatures are calculated according to the formula (2), taking into account that the mercury molar mass $\mu = 200.59 \cdot 10^{-3} \frac{\text{kg}}{\text{mole}}$, the interatomic porosity $K_{na} = 0.4$. The following radius values are calculated as a

result: $r = 3.2503 \cdot 10^{-10} \text{ m}$ at $t = -39.9^\circ\text{C}$, $r = 3.321 \cdot 10^{-10} \text{ m}$ at $t = 0^\circ\text{C}$, $r = 3.597769 \cdot 10^{-10} \text{ m}$ at $t = 800^\circ\text{C}$. The mercury atom radii calculated using density values at three temperature states are consistent with the quantitative assessment of the mercury atom radii of the wavelength range $\lambda = (17109.93 \div 15295.82) \text{ \AA}$, (the spectrum used in calculations is $142 \div 15295.82 \text{ \AA}$, (the spectrum used in calculations corresponds to 142 photons,

with the range of emitted waves from $\lambda_{\max} = 45122.04 \text{ \AA}$ to $\lambda_{\min} = 1250.59 \text{ \AA}$). The radius of the mercury atom in this wavelength range varies from $r_{\max} = 9.4969 \text{ \AA}$ to $r_{\min} = 0.1847 \text{ \AA}$.

TABLE II. CALCULATION OF MERCURY ATOM RADII ACROSS THE WHOLE RANGE OF ENERGY STATES (PART 1)

№	Element	I Electron				Atom radius, Å				
		$\lambda_{\min}, \text{\AA}$	$\lambda_{\max}, \text{\AA}$	$r_{\min}, \text{\AA}$	$r_{\max}, \text{\AA}$	<i>Data by [14]</i>	<i>By Pauling [12]</i>	<i>By Melvin Hughes [12]</i>	<i>By Belov and Bokita [2]</i>	<i>From the Periodic Table [22]</i>
1	2	3	4	5	6	7	8	9	10	11
1	Hydrogen	911.754	388592.7	0.1683	71.734	0.79	0.31	0.3707	0.46	---
2	Helium	320.392	21132.04	0.0473	3.1212	0.49	---	0.53	1.22	---
3	Lithium	2333.93	68580.17	0.3447	10.129	1.57	1.34	1.52	1.55	1.57
4	Beryllium	1426.11	31778.70	0.2106	4.6937	1.13	1.07	1.113	1.13	1.13
5	Bohr	993.38	36010.65	0.1467	5.3187	0.97	0.89	0.795	0.91	0.97
6	Carbon	945.191	25842.20	0.1396	3.8168	0.77	0.77	0.771	0.77	0.77
7	Nitrogen	612.883	18751.01	0.0905	2.7695	0.71	0.70	0.547	0.71	0.71
8	Oxygen	679.202	26173.56	0.1003	3.8658	0.74	0.66	0.6037	---	0.74
9	Fluorine	680.698	11557.17	0.1005	1.7069	0.64	0.64	0.709	---	---
10	Neon	576.00	40575.72	0.0850	5.9930	1.6	---	1.60	1.60	1.60
11	Sodium	2464.77	40431.88	0.3640	5.9717	1.86	1.54	1.858	1.89	1.86
12	Magnesium	1625.22	26392.90	0.2400	3.8982	1.6	1.40	1.599	1.60	1.60
13	Aluminum	1181.807	21163.75	0.1745	3.1258	1.43	1.26	1.432	1.43	1.43
14	Silicon	1255.276	26644.44	0.1854	3.9353	1.18	1.17	1.176	1.34	1.18
15	Phosphorus	1241.49	20590.73	0.1833	3.0412	1.3	1.10	0.947	1.30	1.30
16	Sulfur	1049.82	34270.76	0.1550	5.0617	1.04	1.04	1.02	---	1.04
17	Chlorine	969.917	40532.16	0.1432	5.9866	---	0.99	0.994	---	---
18	Argon	797.744	40880.07	0.1178	6.0379	1.92	---	1.92	1.92	1.92
19	Potassium	653.31	85100.0	0.0964	12.569	2.36	---	2.272	2.36	2.36
20	Calcium	2150.78	19932.94	0.3176	2.9440	1.97	---	1.974	1.97	1.97
21	Scandium	2706.78	7800.44	0.3997	1.1521	1.62	---	---	1.64	1.62
22	Titanium	2273.28	11403.89	0.3357	1.6843	1.46	---	1.44	1.46	1.46
23	Vanadium	1957.90	11107.7	0.2891	1.6406	1.31	---	1.32	1.34	1.31
24	Chrome	1999.95	11610.48	0.2953	1.7148	1.27	1.25	1.249	1.27	1.27
25	Manganese	1996.06	17607.50	0.2948	2.6006	1.30	---	1.366	1.30	1.30
26	Iron	1855.58	11973.07	0.2740	1.7684	1.26	---	1.241	1.26	1.26
27	Cobalt	1847.89	11630.93	0.2729	1.7178	1.25	1.24	1.246	1.24	1.25
28	Nickel	2014.25	18040.6	0.2975	2.6646	1.24	1.24	1.246	1.24	1.24
29	Copper	1713.36	18229.0	0.2530	2.6924	1.28	1.35	1.278	1.28	1.28
30	Zinc	809.92	7799.37	0.1196	1.1519	1.37	1.31	1.333	1.39	1.37
31	Gallium	1505.6	12109.93	0.2223	1.7886	1.39	---	1.221	1.39	1.39
32	Germanium	1143.25	20673.64	0.1688	3.0534	1.39	---	1.149	1.39	1.39
33	Arsenic	1515.48	10888.82	0.2238	1.6082	1.48	1.21	1.248	1.48	1.48
34	Selenium	1377.98	10386.28	0.2035	1.5340	1.6	---	1.16	1.60	1.60
35	Bromine	1101.5	22865.65	0.1629	3.3772	1.19	1.14	1.141	---	1.19
36	Krypton	862.36	30979.22	0.1273	4.5756	1.98	---	1.97	1.98	1.98
37	Rubidium	3023.66	27905.37	0.4465	4.1216	2.48	---	2.475	2.48	2.48
38	Strontium	2428.1	30110.0	0.3586	4.4472	2.15	---	2.151	2.15	2.15
39	Yttrium	2813.64	10683.4	0.4155	1.5779	1.81	---	---	1.81	1.81
40	Zirconium	2285.25	10210.44	0.3375	1.5080	1.6	---	1.59	1.60	1.60
41	Niobium	2211.46	10563.7	0.3266	1.5602	1.45	---	---	1.45	1.45
42	Molybdenum	2471.97	8389.32	0.3651	1.2391	1.40	1.40	1.363	1.39	1.40

TABLE III. CALCULATION OF MERCURY ATOM RADII ACROSS THE WHOLE RANGE OF ENERGY STATES (PART 2)

№	Element	I Electron				Atom radius, Å				
		$\lambda_{min}, \text{\AA}$	$\lambda_{max}, \text{\AA}$	$R_{min}, \text{\AA}$	$R_{max}, \text{\AA}$	Data by [14]	By Pauling [12]	By Melvin, Hughes [12]	By Belov and Bokitaia [12]	From the Periodic Table [22]
43	Technetium	2376.05	8829.8	0.3509	1.3041	1.36	---	---	1.39	1.36
44	Ruthenium	2076.43	8264.95	0.3066	1.2207	1.34	---	1.34	1.34	1.34
45	Rhodium	2264.14	9757.11	0.3344	1.4411	1.37	---	1.35	1.34	1.37
46	Palladium	1890.41	10890.26	0.2792	1.6084	1.37	1.37	1.376	1.37	1.37
47	Silver	1507.37	39951.0	0.2226	5.9007	1.44	1.53	1.445	1.44	1.44
48	Cadmium	701.20	39087.0	0.1035	5.7731	1.56	1.48	1.49	1.56	1.56
49	Indium	1648.0	16748.0	0.2434	2.4736	1.66	---	1.626	1.66	1.66
50	Tin	1804.6	13608.0	0.2665	2.0099	1.58	1.40	1.40	1.58	1.58
51	Antimony	1456.62	12116.06	0.2151	1.7895	1.61	1.41	1.45	1.61	1.61
52	Tellurium	1700.0	10149.2	0.2510	1.4990	1.7	---	1.35	1.70	1.70
53	Iodine	1259.15	16038.15	0.1859	2.3688	1.36	1.33	1.3313	---	1.36
54	Xenon	952.1	26511.0	0.1406	3.9156	2.18	---	2.18	---	2.18
55	Cesium	3288.61	68070.0	0.4857	10.054	2.62	---	2.655	2.68	2.62
56	Barium	2133.58	30933.8	0.3151	4.5689	2.24	---	2.174	2.21	2.24
57	Lanthanum	3215.81	10612.56	0.4749	1.5674	1.87	---	1.87	1.87	1.87
58	Cerium	3437.81	8891.2	0.5077	1.3132	1.82	---	1.825	1.83	1.82
59	Praseodymium	2488.75	8854.05	0.3675	1.3077	1.82	---	---	1.82	1.82
60	Neodymium	4337.22	6846.72	0.6406	1.0112	1.82	---	---	1.82	1.82
61	Promethium	2502.12	8335.63	0.3695	1.2311	---	---	---	---	---
62	Samarium	3687.88	8913.66	0.5446	1.3165	1.8	---	---	1.81	1.80
63	Europium	2709.99	7887.98	0.4002	1.1650	2.04	---	---	2.02	2.04
64	Gadolinium	2892.08	8668.63	0.4271	1.2803	1.79	---	---	1.79	1.79
65	Terbium	3558.77	6896.37	0.5256	1.0185	1.77	---	---	1.77	1.77
66	Dysprosium	2585.3	10523.39	0.3818	1.5543	1.77	---	---	1.77	1.77
67	Holmium	3424.11	8915.98	0.5057	1.3168	1.76	---	---	1.76	1.76
68	Erbium	3368.18	9927.1	0.4974	1.4662	1.76	---	1.86	1.75	1.76
69	Thulium	2596.49	8017.9	0.3835	1.1842	1.75	---	---	1.74	1.75
70	Ytterbium	2464.5	10770.1	0.3640	1.5907	1.93	---	---	1.93	1.93
71	Lutetium	2685.08	24170.0	0.3965	3.5699	---	---	---	1.74	---
72	Hafnium	2845.83	10637.93	0.4203	1.5712	1.59	---	1.61	1.59	1.59
73	Tantalum	2396.3	10099.41	0.3539	1.4916	1.46	---	---	1.46	1.46
74	Tungsten	2098.25	8613.26	0.3099	1.2721	1.41	---	1.371	1.40	1.41
75	Rhenium	1716.45	10639.45	0.2535	1.5714	1.37	---	---	1.37	1.37
76	Osmium	2001.45	7602.95	0.2956	1.1229	1.36	---	1.338	1.35	1.36
77	Iridium	2010.63	7183.71	0.2969	1.0610	1.36	---	---	1.35	1.36
78	Platinum	1969.69	8762.47	0.2909	1.2942	1.39	1.38	1.388	1.38	1.39
79	Gold	1578.24	9391.7	0.2344	1.3871	1.44	1.50	1.442	1.44	1.44
80	Mercury	1250.59	45122.04	0.1847	6.6645	1.57	1.48	1.503	1.60	1.57
81	Thallium	1489.65	21802.17	0.2200	3.2201	1.71	---	1.704	1.71	1.71
82	Lead	1722.66	10969.53	0.2544	1.6201	1.75	1.46	1.75	1.75	1.75
83	Bismuth	1489.94	22554.2	0.2200	3.3312	1.82	1.51	1.548	1.82	1.82
84	Polonium	1919.4	9374.8	0.2834	1.3846	1.19	---	---	---	1.19
85	Astatine	2162.25	2244.01	0.3193	0.3314	---	---	---	---	---
86	Radon	1451.56	9327.02	0.2143	1.3776	1.34	---	---	---	1.34
87	Francium					---	---	---	2.80	---
88	Radium	3101.8	9932.21	0.4581	1.4669	---	---	---	2.35	---
89	Actinium	2968.82	7866.10	0.4384	1.1618	---	---	---	2.03	---
90	Thorium	2891.25	10875.05	0.4270	1.6062	1.80	---	---	1.80	1.80
91	Protactinium	2522.61	4433.44	0.3725	0.6548	---	---	---	1.62	---
92	Uranium	3027.66	21911.0	0.4471	3.2362	1.20	---	1.49	1.53	1.20
93	Neptunium	2655.0	4363.8	0.3921	0.6445	---	---	---	1.50	---
94	Plutonium	2477.0	21126.0	0.3953	3.1203	---	---	---	1.62	---
95	Americium	2953.71	8497.82	0.4362	1.2551	---	---	---	---	---
96	Curium	2516.0	4989.9	0.3716	0.7370	---	---	---	---	---
97	Berkelium	3412.01	3916.24	0.5039	0.5784	---	---	---	---	---
98	Californium	3706.4	4335.2	0.5474	0.6403	---	---	---	---	---
99	Einsteinium	3065.4	6539.71	0.4527	0.9659	---	---	---	---	---
100	Fermium	---	---	---	---	---	---	---	---	---
101	Mendelevium	---	---	---	---	---	---	---	---	---

In the same way it is possible to calculate atom radii for different elements given that their density and a crystal lattice type, which determines the interatomic porosity, are known. A similar method for calculating the radii of atoms was used by Pauling, Melvin-Hughes, Belov and Bokia [12], whose data for many elements slightly differ, probably since they used different values of the coordination number. However, it is difficult to calculate atom radii for different elements using values of their bulk density in a wide range of temperatures (energy states) since there are no data on their density and crystal lattice types under these conditions.

The formula (3) was used to assess the minimum and the maximum atom radii for all chemical elements based on threshold values of wavelengths of photon emission (absorption) and spectrum data for these chemical elements [25, 26]. The calculated results of threshold values of the atom radii are shown in Table 2.

If analyzed, this table shows that for 75% of elements data on atom radii provided by different authors fit into the range ($r_{\min} - r_{\max}$), which is calculated using using threshold values of wavelengths of photon emission-absorption. In comparison to others, for the first 18 elements more recent information on the atom spectrum was used. It allowed for more objective data on their atom radius threshold values.

The greatest number of discrepancies between values calculated based on spectral analysis data ($r_{\min} - r_{\max}$) and data on the atom radii of elements provided by other authors (Table 2) is found for lanthanoid elements. It can be explained by the fact that the spectral analysis data on these and a number of other elements are not complete enough. Such conclusion is confirmed by comparing threshold values of wavelengths for emission-absorption from earlier [25] and later [26] publications for the first 18 elements.

This approach allows for objective assessment of atom radii of chemical elements across the entire range of their energy state, i.e. a wide range of temperatures. Thus, using the proposed method, we have calculated the atom radii for all chemical elements across their entire energy state range, which distinguishes this work from those of other authors (V. Brattsev [16], A. Radtsig and V. Shustriakov [22], L. Pauling [12], N. V. Belov and G. [12], etc.), the data of which correspond to a certain narrow range of temperature corresponding to normal conditions.

CONCLUSION

1. In this research we provided assessment of the threshold values range ($r_{\min} - r_{\max}$) of atom radii for all chemical elements of the periodic table. It is shown that data on atom radii calculated using threshold values of wavelengths of photon emission-absorption in most cases coincide with the experimental (reference) provided by different authors. For a number of chemical elements, especially heavy ones, data on the change ranges of the atom radii is published for the first time.
2. There is a satisfactory correspondence between values of atom radii calculated based on emitted photon

energy and ones calculated using a traditional approach, i.e. via the substance density. It validates the proposed methodological approach to the assessment of atom radii across their entire energy range.

3. The expected decrease of atom radii by photon emission confirms the existence of a photon electromagnetic field around atom electrons and proton-electron-photon model of the atom.

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